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# Nuclear structure calculations with a sum of Sussex interaction and 3-body delta force : binding energies of closed-shell nuclei

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The Sussex matrix elements lack saturation property because of the missing short-range strong repulsion. We demonstrate here that the 3-body repulsive delta force may be used to simulate the effect of the short-range repulsion. When the delta force is added to the Sussex interaction the results are almost identical with those obtained earlier by first calculating a $G$-matrix from the hard core and then adding this to the old Sussex matrix elements.

## 1. Introduction

Some time in the past Elliott *et al* (1968) deduced a restricted set of matrix elements (Sussex matrix elements or SME) of the nucleon-nucleon interaction directly from the nucleon-nucleon phase shifts without specifying the potential. In a later paper Dey *et al* (1969) used these matrix elements to make first order calculations of binding energies and spectra at or near closed shells. It was shown that though sensible results were obtained when the oscillator length parameter $b$ was chosen to give the right size of the nucleus, these matrix elements did not have the necessary saturation property. The minimum of the binding energy curve occurred, if at all, at a very small value of $b$

Still later a technique for adding the effect of a short-range repulsion to the SME was developed by Sanderson *et al* (1974) In the relative $s$-state the actual nucleon-nucleon potential was assumed to be the sum of a smooth potential implied by the SME and an essentially hard core (central, spin-independent) potential containing a few parameters. These parameters (except the core radius) were chosen such that the phase shifts due to the entire potential were practically the same as due to the smooth part alone The fitting was done for different values of the core radius. A $G$-matrix was then calculated from the *hard core part* of the potential only The $G$-matrix elements were used in conjunction with the old Sussex matrix elements to calculate the binding energies and spectra of various nuclei. Hereafter this combination of the $G$-matrix and the Sussex matrix elements will be referred to as the *modified* Sussex matrix elements (MSME). Due to the presence of the $G$-matrix, calculations with MSME did lead to saturation. The core radius was chosen to give reasonable values of

the binding energies at the correct value of $b$ for a number of nuclei. Due to the simple form of the additional potential it is not too difficult to solve the Bethe-Goldstone equation. However, it is still far from being simple. Therefore it might be worthwhile to find a simple substitute for the Sussex $G$-matrix

Skyrme (1959), Vautherin & Brink (1972), Sharp & Zamick (1973) and many others have used the 3-body delta force as a constituent of phenomenological forces to achieve saturation. As Vautherin & Brink (1972) have pointed out this force owes its origin (in parts) to the strong short-range repulsion. That a sum of a repulsive 3-body delta force and a reasonable, overall attractive force will lead to saturation is guaranteed. This is so because the contribution of the delta force is inversely proportional to the sixth power of $b$. This is much faster than the variation in the attractive contribution of the other part of the force. Hence by varying the strength of the 3-body delta force one can always get the minimum of the binding energy curve at the desired value of $b$

In the present paper we wish to investigate the consequences of the following assumption . The $G$-matrix part of the MSME which is entirely due to the hard core may be effectively replaced by the 3-body delta force with the proviso that. that part of the delta force which cannot be reduced to an effective 2-body force will not be included and Brueckner type diagrams will be ignored An example where the 3-body delta force cannot be reduced to an effective 2-body force is the $3p$–$3h$ contribution to the binding energy of a closed—shell nucleus.

It must be stressed that this is not yet another purely phenomenological calculation. The main part of the interaction is still realistic (in the sense that it has been derived from the $N$–$N$ phase shifts). There is no parameter of any kind in this part of the force. However, we treat the strength of the 3-body delta force as a variational parameter. It may be mentioned that the Sussex $G$-matrix which we are replacing also has a parameter, namely, the hard core radius.

Just how useful this replacement of the hard core by the above effective force is can only be judged by results. The first aim of this calculation is to investigate whether saturation can be achieved for different nuclei at the correct value of $b$ with the same or nearly the same value of the strength constant. Our second aim is to examine the behaviour of this force in second order of perturbation theory and compare the results with those calculated with the MSME. In the present paper we have calculated the binding energies of several closed-shell nuclei to first order and of $^{16}O$ to second order of perturbation theory Oscillator wave functions are used and the centre of mass motion has been handled in the same way as by Sanderson *et al* (1974). The single particle energies needed to calculate the energy denominators have been taken from the above reference.

In sec. 2 we explain how the coupled matrix elements of the 3-body delta force are evaluated. The details of the Hamiltonian are also given. Sec. 3 is devoted to the discussion of diagrams. In Sec. 4 we present the results of the first order calculation. The second order results are presented in Sec. 5. Only *LS* closed-shell nuclei with $N = Z$ are studied here

## 2 Matrix Elements of the Delta Force

In the second-quantised notation a 3-body interaction can be written as

$$V_3 = \frac{1}{3!} \Sigma < klm \,|\, V_3 \,|\, pqr > a_k^+ a_l^+ a_m^+ a_r a_q a_p \qquad \ldots \quad (1)$$

where $k$, $l$, etc represent *all* quantum numbers of the single-particle states of the chosen basis (oscillator states in the present work). It is convenient to define an *antisymmetrised* coupled matrix element

$$< \gamma_1 \gamma_2(\Gamma_{12})\gamma_3 \Gamma \,|\, V_3 \,|\, \gamma_4 \gamma_5(\Gamma_{45})\gamma_6 \Gamma >_a$$

$$= < \gamma_1 \gamma_2(\Gamma_{12})\gamma_3 \Gamma \,|\, V_3 \,|\, a\{\gamma_4 \gamma_5(\Gamma_{45})\gamma_6 \Gamma\} > \qquad \ldots \quad (2)$$

where $a$ is the antisymmetrising operator. In eq. (2) $\gamma_1$ etc. stand for all the labels necessary to specify the single-particle states. $\Gamma_{12}$, $\Gamma$ etc stand for the set of intermediate and total angular momenta and isospins which are needed to specify the coupled 3-particle states. For the $jj$ coupled states $\Gamma$ stands for $J$ and $T$ whereas in $LS$ coupling it stands for $L$, $S$, and $T$

When expressions for various diagrams (except for the $3p$–$3h$ case, which anyway we are not considering) are deducted one meets the sum

$$\sum_{\Gamma,\eta} (2\Gamma+1) < \gamma_1\gamma_2(\Gamma_{12})\eta\Gamma \,|\, V_3 \,|\, \gamma_4\gamma_5(\Gamma_{45})\eta\Gamma >_a^{(3)} \qquad \ldots \quad (3)$$

where $\eta$ stands for the single-particle states of the core. Hence it is convenient to define an effective 2-body interaction whose matrix elements are given by

$$(2\Gamma_{12}+1) < \gamma_1\gamma_2\Gamma_{12} \,|\, \hat{V}_2 \,|\, \gamma_4\gamma_5\Gamma_{12} >_a = \frac{1}{3} \sum_{\eta,\Gamma} (2\Gamma+1)$$

$$\times < \gamma_1\gamma_2(\Gamma_{12})\eta\Gamma \,|\, V_3 \,|\, \gamma_4\gamma_5(\Gamma_{12})\eta\Gamma >_a. \qquad \ldots \quad (4)$$

The factor 1/3 is arbitrary. Since $V_2$ may be shown to be equivalent to a density-dependent force the factor has been chosen to agree with the convention used by workers using density-dependent forces.

In the present work the 3-body interaction is given by :

$$V_3 = t_3\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta(\boldsymbol{r}_2-\boldsymbol{r}_3)$$

$$= \frac{3\sqrt{3}\pi^3}{4}\beta\delta(\boldsymbol{r}_1-\boldsymbol{r}_2)\delta(\boldsymbol{r}_2-\boldsymbol{r}_3)$$

$$\left(\frac{3\sqrt{3}\pi^3}{4} \simeq 40{\cdot}3\right) \qquad \ldots \quad (5)$$

where $\beta$ is a positive constant related to the $t_3$ of Skyrme (1959) Since this force is independent of spin or isospin it is convenient to work with $LS$ coupled states. It can be shown that :

$$< \gamma_1\gamma_2(L_{12}S_{12}T_{12})\gamma_3 LST \mid V_3 \mid \gamma_4\gamma_5(L_{45}S_{45}T_{45})\gamma_6 L'S'T' >_a$$

$$= \delta_{LL'}\,\delta_{SS'}\,\delta_{TT'}\,\delta_{S\frac{1}{2}}\,\delta_{T\frac{1}{2}}\,\delta_{S_{12}S_{45}}\,\delta_{T_{12}T_{45}}\left(\frac{1-(-1)^{S_{12}+T_{12}}}{2}\right)$$

$$\times(-1)^{L_{12}+L_{45}}\,[3\;4\;L_{12}L_{45}]^{\frac{1}{2}}\begin{pmatrix} l_1 & l_2 & L_{12} \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} L_{12} & l_3 & L \\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} l_4 & l_5 & L_{45} \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times\begin{pmatrix} L_{45} & l_6 & L \\ 0 & 0 & 0 \end{pmatrix} I(n_1l_1, n_2l_2, n_3l_3, n_4l_4, n_5l_5, n_6l_6)\beta/b^6 \qquad (6)$$

where a factor, say $b$, inside a pair of square brackets represents $(2b+1)$ and

$$I(n_1l_1, n_2l_2, n_3l_3, n_4l_4, n_5l_5, n_6l_6)/b^6$$

$$= \frac{3\sqrt{3}\pi}{16}\,[l_1l_2l_3l_4l_5l_6]^{\frac{1}{2}}\int_0^\infty\left[\prod_{i=1}^{6}R_{n_il_i}(r)\right]r^2dr. \qquad \ldots \quad (7)$$

$R_{nl}$ is the radial part of the oscillator wave function as defined by Elliott *et al* (1968) Eq (6) can be deduced by expressing a coupled product of two spherical harmonics of the *same* argument in terms of a single spherical harmonic of the same argument (see Satchler & Brink 1968). The matrix elements are non-zero only if the space part of the 3-particle states are completely symmetric which in turn implies that the spin-isospin part must be completely antisymmetric As is well known, (see for example Hamermesh 1964), such a state must have $T = S = 1/2$. A similar argument leads to the restriction that the sum of

$T_{12}$ and $S_{12}$ must be equal to one. The matrix elements of the equivalent 2-body interaction are given by .

$$< \gamma_1\gamma_2 LST \,|\, \hat{V}_2 \,|\, \gamma_3\gamma_4 LST >_a$$

$$= \left(\frac{1-(-1)^{S+T}}{2}\right) \frac{1}{3} \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_3 & l_4 & L \\ 0 & 0 & 0 \end{pmatrix}$$

$$\times \sum_{\beta} I(n_1 l_1, n_2 l_2, n_3 l_3, n_4 l_4, n_h l_h, n_h l_p)\beta / b^6. \qquad (8)$$

Except for a numerical factor it is *these* matrix elements which replace the $G$-matrix elements. Since we want to work with $jj$ coupled states the 2-body effective matrix elements are calculated by applying the usual transformation. The radial integral occuring in eqs. (7) and (8) may be reduced to a sum of terms involving Gamma functions of half-integral order. The $b$-dependence has been removed from $I$

In the present calculation we consider the following hamiltonian :

$$H = T + V_2 + V_3 + \frac{1}{2} mA\omega^2 R^2 \qquad (9)$$

in which $T$ is the kinetic energy operator of the $A$-nucleon system, $V$ is the smooth potential implied by the SME, $V_3$ is defined by eq. (5), and the last term represents an oscillator potential on the centre of mass coordinates $R = \sum_i r_i/A$ The reason for adding the last term has been fully explained by Sanderson *et al* (1974). The unperturbed Hamiltonian is taken to be a sum of single-particle oscillators with shifted energies as in the last reference .

$$H_0 = H_{0sc} + \Lambda \qquad \ldots \quad (10)$$

where

$$\Lambda = \sum_{nlj} \lambda_{nlj} \,|\, nlj > < nlj \,| \qquad \ldots \quad (11)$$

The perturbation $H_0$ is the difference between $H$ and $H_0$ and may be written as

$$H_1 = V_2 + V_3 - \Lambda \qquad \ldots \quad (12)$$

as was done by Sanderson *et al* (1974), where

$$V_2 = V_2 - \sum_{i<j} \frac{m\omega^2}{2A} (r_i - r_j)^2 \qquad \ldots \quad (13)$$

is the two body part of the perturbation. If $3p$–$3h$ diagrams are ignored $V_3$ may be shown to be equivalent to $\alpha \hat{V}_2$ where $\hat{V}_2$ is defined by eq (8) and p is a simple factor which depends upon the nature of the vertex on which $\hat{V}_2$ is acting.

There is no dependence on $\lambda_{ntj}$ up to the first order. In second order the only effect is through the energy denominators. We have used the energy shifts calculated by Sanderson *et al* (1974). All the single-particle oscillator levels are pushed down though the wave functions are not affected. The displacement is quite large for the occupied state and gradually decreases as we move to higher oscillator levels. This has the effect of increasing the energy denominators. Sanderson *et al* (1974) have argued that such a single-particle spectrum helps to reduce both the second order attractive and the third order repulsive contributions thus improving the convergence of the perturbation theory.

## 3. Diagrams

The 3-body diagrams are too unwieldly to draw on paper The expressions given in the appendix have been deduced by using the standard second-quantised technique *directly*. Since in diagrams involving the 3-body force (except the $3p$–$3h$ case) there is always at least one Hartree-Fock bubble at the 3-body vertex the corresponding expressions contain a sum over the single-particle states of the core and also over the total 3-particle angular momentum and isospin. After performing these sums the expressions reduce to those with an effective 2-body force $\hat{V}_2$ except for some simple numerical factors Except for the extra factor the 3-body vertices in which we are interested may always be replaced by a 2-body vertex with the effective 2-body interaction $\hat{V}_2$ In figure 1 the diagrams have been drawn after this replacement. The actual 2-body interaction $\hat{V}_2$ is represented by broken lines and the effective 2-body interaction by solid lines. The numerical factor $\alpha$ by which the matrix elements of $\hat{V}_2$ are to be multiplied are shown next to the vertex concerned We offer the following generalisation if $\hat{V}_2$ acts on a vertex which has two, one or no Hartree-Fock bubble the factor $\alpha$ is 1, 3/2 or 3 respectively This is in agreement with the conclusions of Sharp & Zamick (1973)

## 4 First Order Results

We present our first order results in the form of graphs for various $LS$ closed-shell nuclei with $N = Z$. Some of the nuclei considered lie far from the stability line. They are included here solely to compare our results with those of Sanderson *et al* (1974) who used MSME Only in the case of $^{16}$O have we shown the variation of binding energy both with and without the effective 2-body force $\hat{V}_2$. The binding energies include the effect of the Coulomb force.

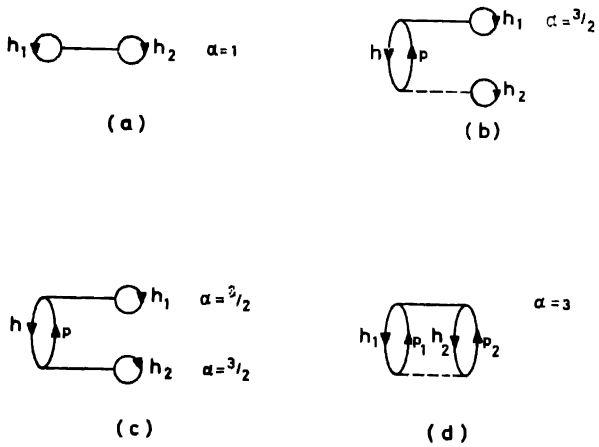


Fig. 1 First and second order graphs obtained by replacing a 3-body vertex by the equivalent 2-body vertex The 2-body interaction $V_2$ has been indicated by a broken line and the effective 2-body interaction $\hat{V}_2$ by a solid line Second order graphs with $V_2$ *only* have not been calculated as their contributions are given by Sanderson *et al* (1974). The numerical factor $\alpha$ is indicated against each of the $\hat{V}_2$ vertices.

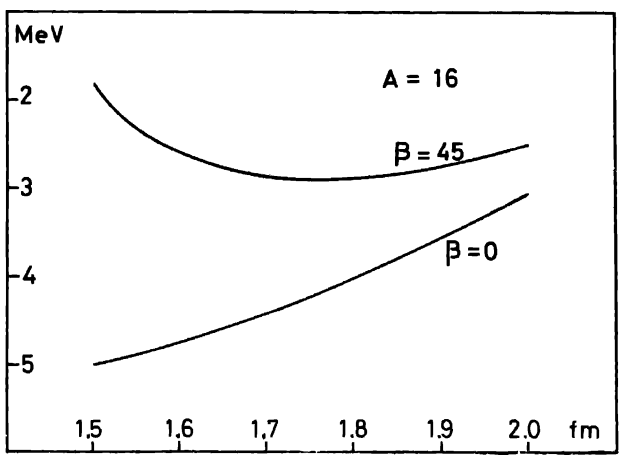


Fig. 2. Binding energy per particle in MeV for $A = 16$ to first order of perturbation theory. The B E. per particle is shown both with and without the effective 2-body interaction $\hat{V}_2$. Coulomb energy is included. $\beta = 45$ MeV fm$^6$.

It can be seen from the graphs (figures 2 and 3) that for $\beta = 45$ MeV fm$^6$ we get the minimum of the binding energy curve in *all* cases at about the same

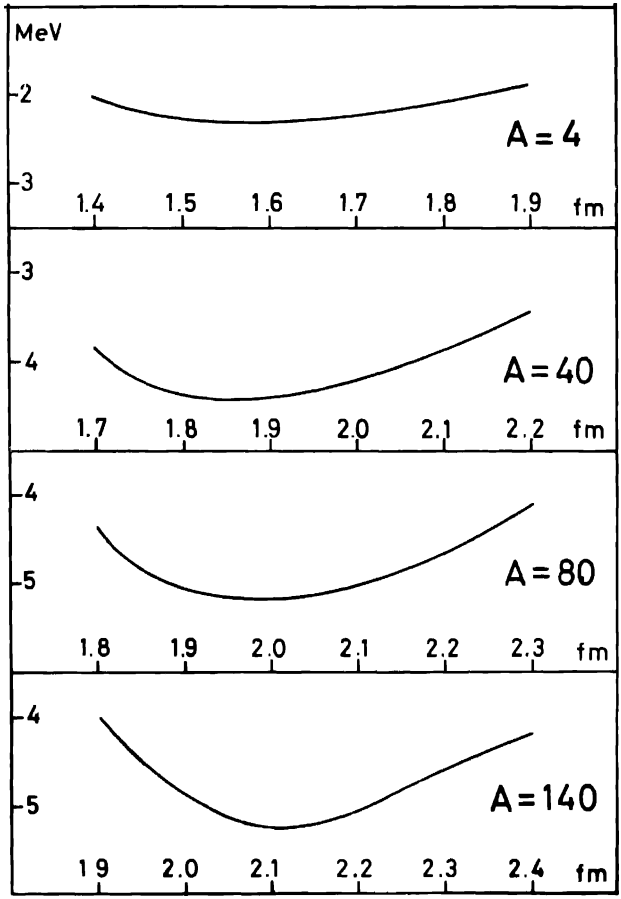


Fig. 3 Binding energy per particle in MeV for $A = 4$, 40, 80 and 140 Coulomb energy is included. $\beta = 45$ MeV fm$^6$

value of $b$ as in the work of Sanderson *et al* (1974). For the case of $^{16}$O at $b = 1{\cdot}7$ fm the contribution of $\hat{V}_2$ with $\beta = 45$ MeV fm$^6$ is about 24 MeV as compared to $-332$ MeV which is the contribution of the original Sussex matrix elements.

This comes to about 7%. The corresponding figures for $^4$He at $b = 1{\cdot}5$ fm are about 4 and $-55$ MeV, and for $^{40}$Ca at $b = 1{\cdot}9$ fm they are 73 MeV and $-1004$ MeV. Again the ratios are nearly 7%. So near the equilibrium value of $b$ the contribution of the effective 2-body force is relatively quite small. The main usefulness of this force is due to the rapid increase in its contribution as we move towards smaller values of $b$. For example, in the case of $^{16}$O changing $b$ from 1·7 to 1·5 fm changes the contribution of the effective 2-body force from 24 MeV to 51 MeV.

The delta force in our calculation is also small compared to that used in purely phenomenological calculations. $\beta = 45$ MeV fm$^6$ corresponds to $t_3 = 1813$ MeV fm$^6$ which should be compared with $t_3 = 8027$ MeV fm$^6$ used by Skyrme (1959). The value used by Vautherin & Brink (1972) is even larger. This means that some of the undesirable effects of the 3-body delta force like antipairing will not be very serious in our case.

With $\beta = 45$ MeV fm$^6$ the equilibrium values of $b$ for $A = 4$, 16 and 40 are nearly 1·55, 1·75 and 1·85 fm respectively. The first one is slightly larger, the second nearly equal and the last slightly smaller than the values which give the correct experimental radii. One may improve the agreement with experiment by allowing $\beta$ to vary slightly with $A$.

## 5 Second Order Calculation

Since the perturbation consists of two terms, second order graphs may be classified into three group. This is similar to the classification adopted by Sanderson *et al* (1974). First we have those graphs in which the 2-body force $V_2$ acts on both the vertices. Then we have the mixed graphs in which $V_2$ and $\hat{V}_2$ act on one vertex each. Lastly we have graphs in which $\hat{V}_2$ acts on both the vertices. For the $2p$–$2h$ case the third type of graph is not included being of Brueckner type. The contribution of the second and third type of graphs is respectively proportional to the first and the second power of $\beta$. Hence, if results for one value of $\beta$ are known results for any other value may be immediately written down. We have taken $\beta = 45$ MeV fm$^6$ in this part of our calculation also. Results are shown in table 1. Intermediate states lying upto 6 $\hbar\omega$ above the unperturbed states have been included. The $1p$–$1h$ contribution decays quickly. Since both the Sussex $G$-matrix and our effective 2-body interaction $\hat{V}_2$ are purely central, only the central part of the SME contributes to the $2p$–$2h$ mixed diagram. As concluded by Sanderson *et al* (1974) this part of SME becomes negligible after $6\hbar\omega$. For example the total contribution of this diagram from intermediate states at energies greater than $6\hbar\omega$ is a mere 0·7 MeV. Hence for the purpose of comparing our calculation with that with MSME it is not necessary to go beyond $6\hbar\omega$.

For ease in comparing our results with those with MSME we have also shown the results of Sanderson *et al* (1974) A glance at this table demonstrate that

Table 1. First and second order contributions of the effective 2-body force $\hat{V}_2$ to the ground state energy of $^{16}$O. The contribution with $V_2$ only has not been shown as it is the same as in Sanderson *et al* (1974). The letters *a*, *b*, *c* and *d* refer to the diagrams of figure 1. The oscillator length constant is 1·7 fm. The energies are in MeV

| | | Present calculation with $\beta$ = 45 MeV fm$^6$ | | | | Calculation with MSME core radius 0·3 fm | | | |
|---|---|---|---|---|---|---|---|---|---|
| | Diagram | 2 $\hbar\omega$ | 4 $\hbar\omega$ | 6 $\hbar\omega$ | total | 2 $\hbar\omega$ | 4 $\hbar\omega$ | 6 $\hbar\omega$ | total |
| I Order | *a* | 24·0 | | | 26·8 | | | | |
| II Order $1p$–$1h$ | *b* | 6 0 | 1·4 | − 0 0 | | 5 3 | 1·1 | 0 0 | |
| | *c* | −3·5 | −0·5 | −0 1 | | −2 9 | −0·3 | 0 0 | |
| total | *b*+*c* | 2 5 | 0·9 | −0 1 | 3·3 | 2·4 | 0·8 | 0 0 | 3·2 |
| $2p$–$2h$ | *d* | 1·7 | 4 3 | 2 6 | 8 6 | 1 5 | 4 2 | 3 1 | 8·8 |
| II order total | | 4 2 | 5 2 | 2·5 | 11·9 | 3 9 | 5 0 | 3·1 | 12·0 |

Results for MSME have been taken from Sanderson *et al* (1974)

there is a very close agreement between the two sets of calculations. In both cases the $1p$–$1h$ contribution dies quickly and the two sets of figures are practically identical For the $2p$–$2h$ case the individual figures are not so close but the total contribution to $6\hbar\omega$ is virtually identical If one ignores fine details one can safely claim that the 2-body effective force $\hat{V}_2$ with $\beta = 45$ MeV fm$^6$ gives results which are quite close to those given by the Sussex $G$-matrix with the core radius $c = 0{\cdot}3$ fm. In fact the agreement in second order is even better than in first order

## 6. Conclusions

We have demonstrated that the effective 2-body force derived from the 3-body delta force has the same effect as the Sussex $G$-matrix at least for binding energy calculations. In other words the short-range repulsion which the SME lack can be simulated by this very simple force. The main attraction of this force is the ease with which its matrix elements can be calculated. The dependence on $b$ and $\beta$ is particularly simple.

As far as the calculation of the single-particle energies of closed-shell+1 nuclei is concerned it is known that in a given major shell the 3-body delta force pushes up a single-particle level with smaller orbital angular momentum relative

to a level with higher orbital angular momentum. For example, 1*s* level (in $^{17}O$) is pushed up relative to the 0*d* levels. This is exactly what we need. When these levels are calculated with SME in first order the relative spacing between the 1*s* and 0*d* levels is of the right sign and magnitude However, when the second order contributions are included the agreement is completely spoiled. The 1*s* level is pulled down by a large amount. It is expected that the 3-body delta force will tend to restore the good agreement. As far as the spectrum of two valence particles is concerned the delta force is expected to give some anti-pairing though on a much reduced scale than in a purely phenomenological calculation. Also it has been suggested by Sanderson *et al* (1974) that one should use a *b* value substantially larger than normally used Such an increase in *b* will reduce the anti-pairing to a large extent because of the inverse sixth-power variation of the matrix elements.

The author wishes to thank Mr. Shtaklef of the A.U.B computer centre for considerable help in computing

## Appendix

In this appendix we list the expressions for those diagrams which contain at least one effective 2-body vertex The letters *a*, *b* etc. refer to the diagrams shown in figure 1

$$E^{(a)} = \frac{1}{2} \sum_{h_1,h_2} \sum_{J,T} [JT] \prec h_1 h_2 JT \,|\, \hat{V}_2 \,|\, h_1 h_2 JT \succ_a \qquad \text{(A-1)}$$

$$E^{(b)} = 2 \sum_{h,p} \delta_{j_h j_p} \left[\frac{1}{2}\, j_h\right]^{-1} (E_h - E_p)^{-1}$$
$$\times \{ \sum_{h_1,J,T'} [JT] \prec h_1 h_2 JT \,|\, V_2 \,|\, p h_1 JT' \succ_a$$
$$\times \left\{ \frac{3}{2} \sum_{h_2 J'T'} [J'T'] < h h_2 J'T' \,|\, \hat{V}_2 \,|\, p h_2 J'T' >_a \right\} \qquad \ldots \text{(A-2)}$$

$$E^{(c)} = \sum_{h,p} \delta_{j_h j_p} \left[\frac{1}{2}\, j_h\right]^{-1} (E_h - E_p)^{-1}$$
$$\times \left\{ \frac{3}{2} \sum_{h_1,J,T} [JT] < h h_1 JT \,|\, \hat{V}_2 \,|\, p h_1 JT >_a \right\}^2 \qquad \ldots \text{(A-3)}$$

$$E^{(d)} = 2 \times \frac{1}{4} \sum_{h_1,h_2 p_1,p_2} \sum_{J,T} [JTj < h_1 h_2 JT \,|\, V_2 \,|\, p_1 p_2 JT >_a$$
$$\times \{3 < h_1 h_2 JT \,|\, \hat{V}_2 \,|\, p_1 p_2 JT >_a\} (E_{h_1} + E_{h_2} - E_{p_1} - E_{p_2})^{-1}. \quad \ldots \text{(A-4)}$$

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